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CHAOTIC OSCILLATIONS IN PVD TECHNOLOGY OF HYDROCARBON MATERIALS

Abstract. Dynamical behavior of damped Morse oscillator driven an external sinusoidal field of gas-discharge electronic gun has been studied as model of molecular system dissociation in PVD.
Key words: model of the dissociation, nonlinear resonances, chaotic oscillation, Morse oscillator with dissipation, PVD technology.

Statement of the Problem. Researchers of metallurgical processes have paid close attention to the crystallization mechanisms in iron alloys. So in [1], are examined the possible mechanisms for the formation of spherical graphite in ductile iron and features of its structure, taking into account the nature of the fullerene iron alloys. In work [2] is identified the molecular form of carbon - the fullerenes C60 - in iron-carbon alloys produced by methods of classical metallurgy, and mechanisms for the formation of fullerenes are shown in the structure of steels and cast irons. These are, first, the formation of fullerenes in the primary crystallization and secondly, the results of structural and phase transformations occurring during thermal influences. Aa a result of research was concluded the role of fullerenes as germ of the grain structure of iron-carbon alloys.

The aim of the work is to develop a mathematical model of the dissociation of hydrocarbon precursor as the first phase of PVD technology under the influence of high-energy electron fluxes for the study the process of formation of fullerenes (molecular crystals formed by fullerenes).

The main part. Electron beams are concentrated sources of energy with high power density (10^8 ... 10^{12}W/m^2), successfully used in electron-beam PVD technology (physical vapor deposition) to obtain film coatings in vacuo. [4]. In the studies to produce steam naphthalene ($C_{10}H_8$) and its molecular dissociation, were used created in NMetAU low vacuum discharge electron guns (NGEP) operating in the pressure range 1 ... 100 Pa.

A characteristic feature of $C_{10}H_8$ is the presence of two benzene rings that can serve as a basis for building a fullerene - truncated icosahedron formed by 20 hexagons 12 pentagons. In addition, the condition for the effective use of precursors in PVD

technology is the low value of the ratio к=H/C [3]. Thus for к(C_2H_2)=1, к(CH_4)=4, at the same time for naphthalene к($C_{10}H_8$)=0,8.

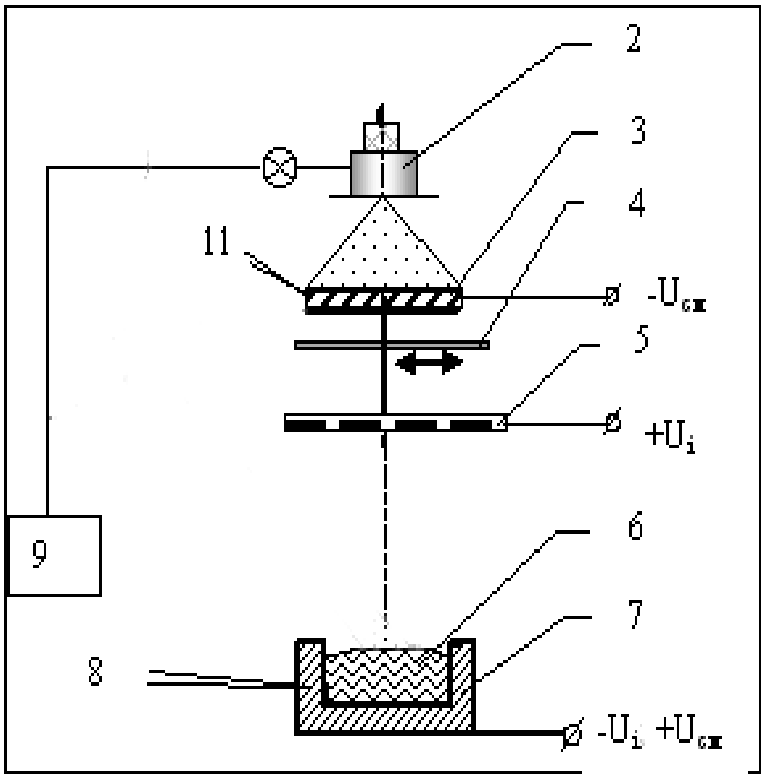
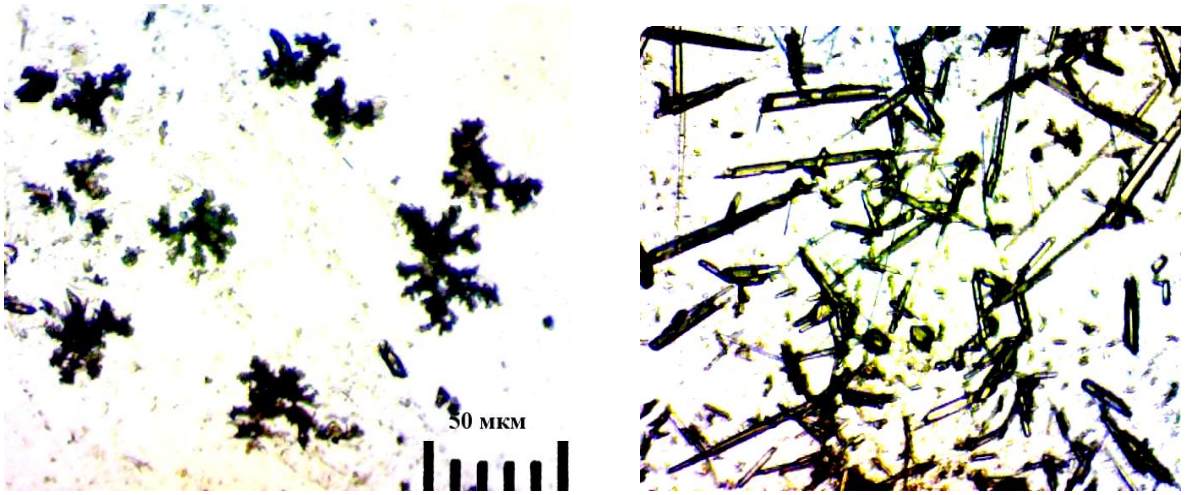


Figure 1 - Schematic of the formation of coatings using NGEP: 2 – NGEP, 3 - substrate, 4 - valve, 5 - ionizer anode, 6 - vaporized material $C_{10}H_8$; 7 - crucible, 8, 11 – thermocouple, 9 - blowing gas system.



а) б)

Figure 2 - Carbon film coating on the glass with a small exposure time: a) fullerites C60, b) needle crystal structures

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Consider the case of use for NGEP $C_{10}H_8$ precursor [4] vapor pressure of P=133Pa, I=0,5, U=5kV, then the concentration of plasma electrons was $n_e \approx 3*10^{11}$ см^3, and the corresponding electron Langmuir frequency of the plasma

$$\omega_e = \sqrt{\frac{4\pi e^2}{m_e} n_e} = 5.64 * 10^4 \sqrt{n_e} \approx 3*10^{10} \text{ с}^{-1} \quad (1)$$

The fullerites are molecular crystals with van der Waals interactions between the molecules C60, forming a three-layer ball densest packing.

For PVD technology interaction model of atoms forming a molecule is based on the concept of molecular dynamics has the form Morse oscillator with dissipation

$$x'' + \gamma x' + (e^{-x} - e^{-2x}) = A\cos\omega\tau, \quad (2)$$

where x - offset relative to the equilibrium position of the atom, ω - the relative frequency of the external force field. Expression (2) describes the nonlinear system, with the possible existence of nonlinear resonances and chaotic oscillation modes □5□. Transition to which causes the accumulation of energy in the external field and the system and as a consequence - the dissociation of molecules.

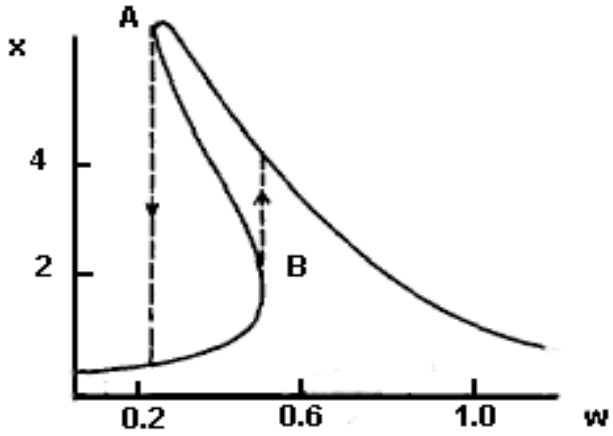

Figure 3 - The dependence of the maximum amplitude of x (1) to the relative frequency of the external force field (non-linear first-order resonance), A and B - cusps hysteresis "fatty" curve - chaotic regimes

A necessary condition for the existence of chaotic oscillations is positive Lyapunov exponent (Fig. 4).

The scenario of transition to chaotic behavior of the system (2) is the process of period-doubling x when changing the control parameter, which in this case is the frequency of the external force field. As a result, a necessary feature of a chaotic mode is the continuous Fourier spectrum of x, limited frequency of the external force field.

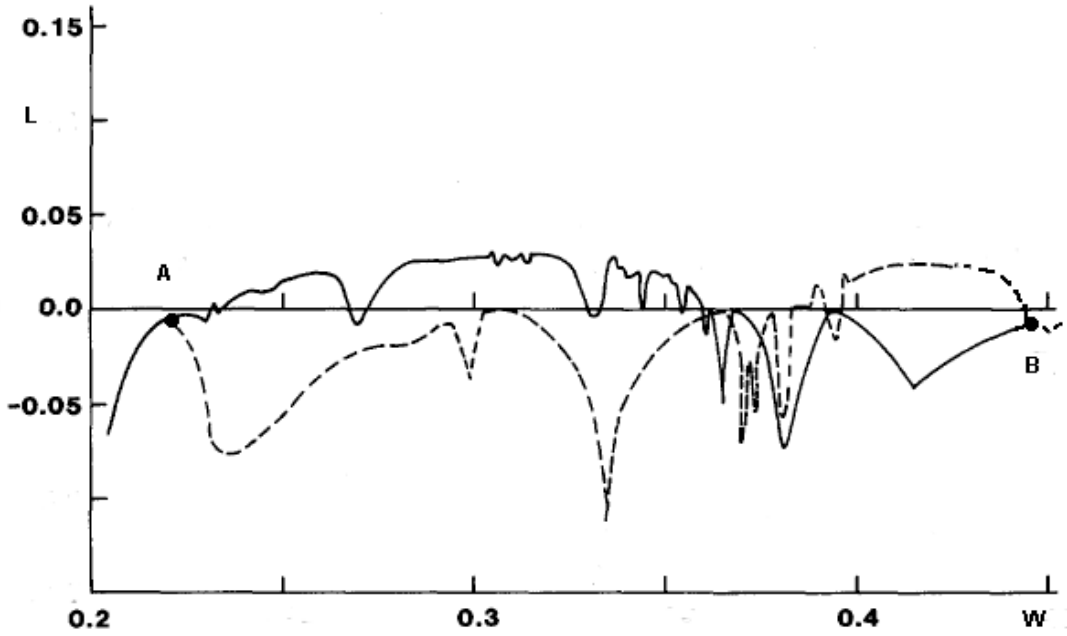

Figure 4 - Dependence of the Lyapunov exponent of the frequency of the external force field: ("solid" line - the bottom line, "dotted" line - upper branch of the hysteresis nonlinear resonance), the coordinates of points A and B = 0.2238 and 0.4412, respectively.

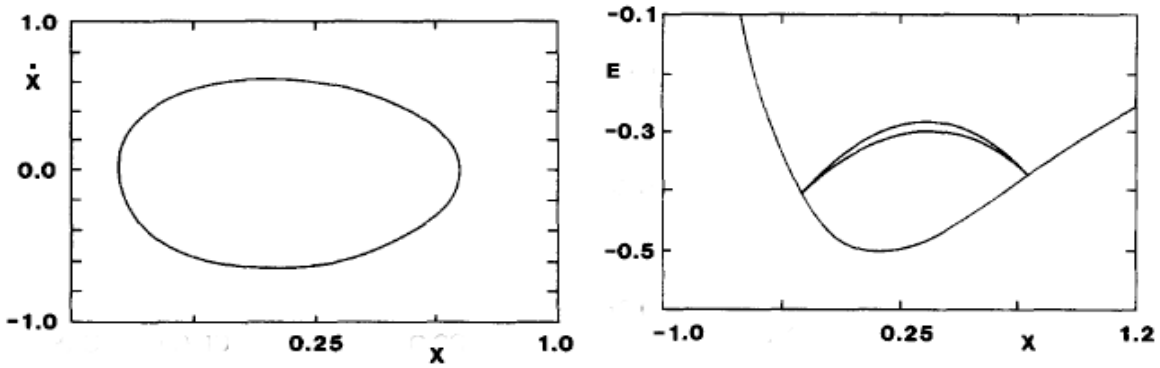

Figure 5 - Harmonic mode of dynamical system (2), a) phase trajectory, b) change in the energy system (2)

Thus, the field of nonlinear resonance (point A) and chaotic modes allocated "fat" line (Fig. 3) differ significantly in various values of x.

The existence of two areas of chaotic modes belonging to one nonlinear resonance (Fig. 3), forms two of dissociation and formation scenario nanocarbon structures (Fig. 2), depending on the growth or decrease of the frequency of the external force field.

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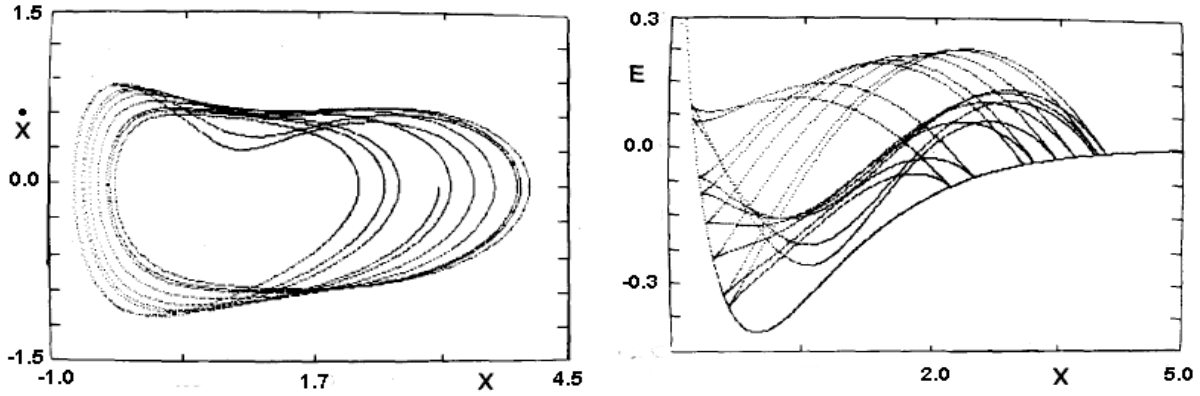

а) б)

Figure 6 - The chaotic mode of the dynamical system (2), a) phase trajectory, b) change in the energy system (2)

Conclusions.

Conducted researches have shown, firstly, the ability of PVD based technologies of low vacuum electron gun discharge, secondly, the existence of the two modes and, respectively, two embodiments of the dissociation process.

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